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Dakota's Role in Verification

Brian Adams

Optimization and Uncertainty Quantification

Russell Hooper

Multiphysics Applications

http://dakota.sandia.gov

CASL Verification Workshop
January 17—19
Albuquerque, NM

DAKOTA
Explore and predict with confidence

CCR
Center for Computing Research

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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REMINDER: WHAT IS DAKOTA?

SNL Mission: Advanced Science and Engineering for National Security

- Nuclear Weapons
- Defense Systems and Assessments
- Energy and Climate
- International, Homeland, and Nuclear Security

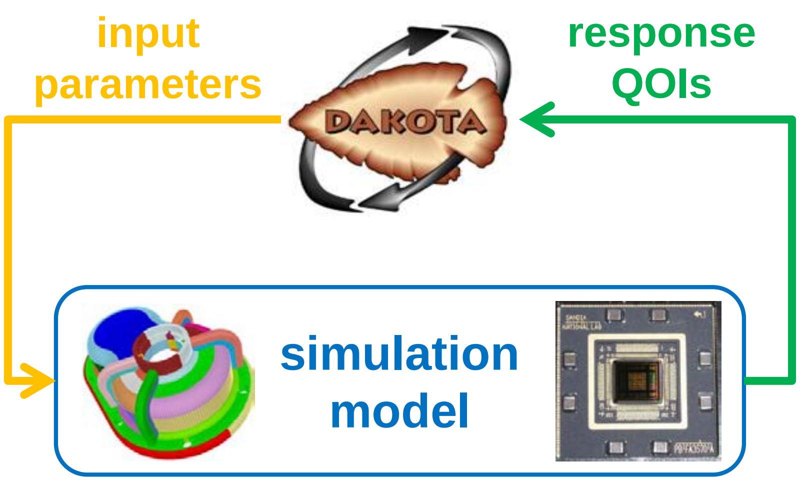
Strong research foundations span many disciplines

Dakota Mission:
To serve Sandia's mission through state-of-the-art research and robust, usable software for optimization and uncertainty quantification.

Dakota Team: has balanced strengths in algorithm research, software design and development, and application deployment and support

Dakota: Algorithms for Design Exploration and Uncertainty Quantification

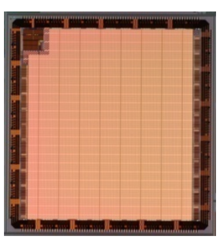
- Suite of iterative mathematical and statistical methods that interface to computational models
- Makes sophisticated parametric exploration of black-box simulations practical for a computational design-analyze-test cycle:
  - Sensitivity Analysis
  - Uncertainty Quantification
  - Design Optimization
  - Model Calibration



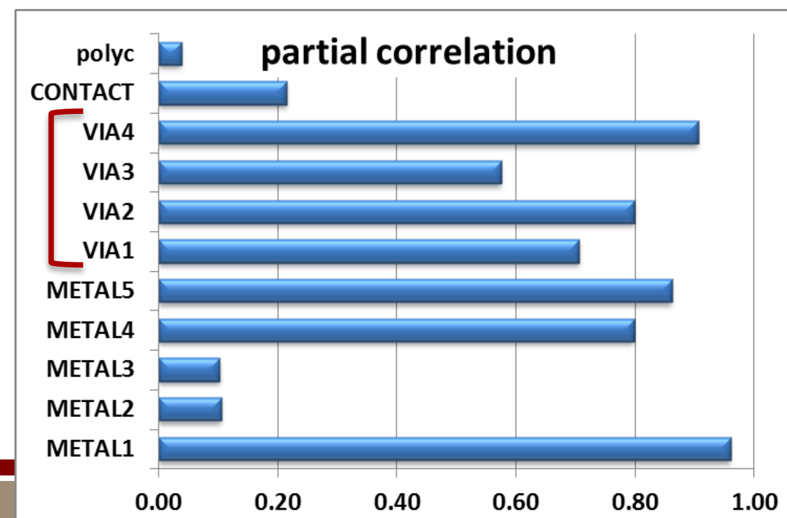
- *Goal: provide scientists and engineers (analysts, designers, decision makers) richer perspective on model predictions*

Sensitivity Analysis

- ***Which are the most influential parameters?***
- Interrogate model to assess input/output mapping
  - Expose model characteristics, trends, robustness
  - Focus resources for data gathering or model/code development
  - Screening: reduce variables for UQ or optimization analysis
- ➢ Dakota automates common single parameter variations, and provides richer global sensitivity methods

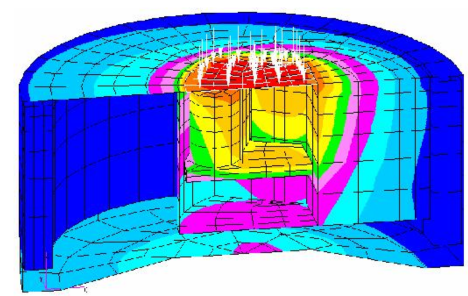


- Xyce model of CMOS7 ViArray
- Assess influence of manufacturing variability on supply voltage performance during photocurrent event

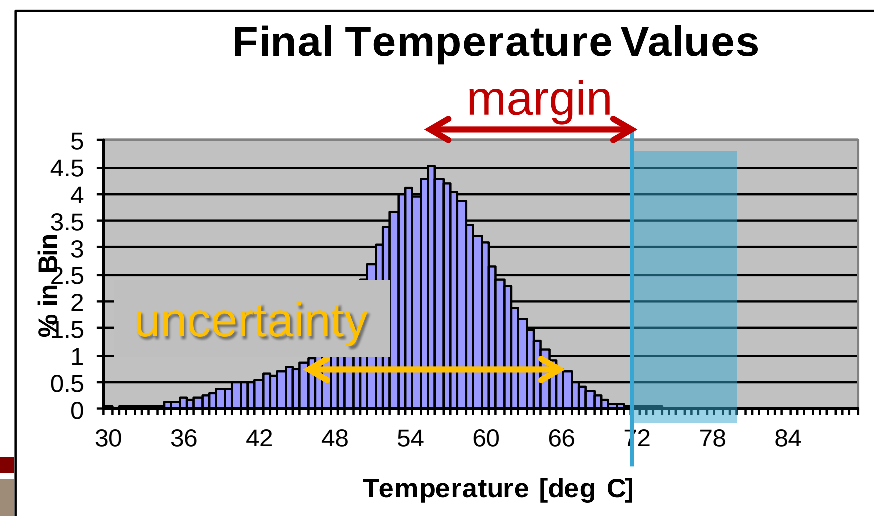


Uncertainty Quantification

- ***Given parameter uncertainty, what is the uncertainty in the model output?***
  - Mean or median performance of a system
  - Overall variability in model response
  - Probability of reaching failure/success (reliability)
  - Range/intervals of possible outcomes
- ➢ UQ also enables statistical validation metrics

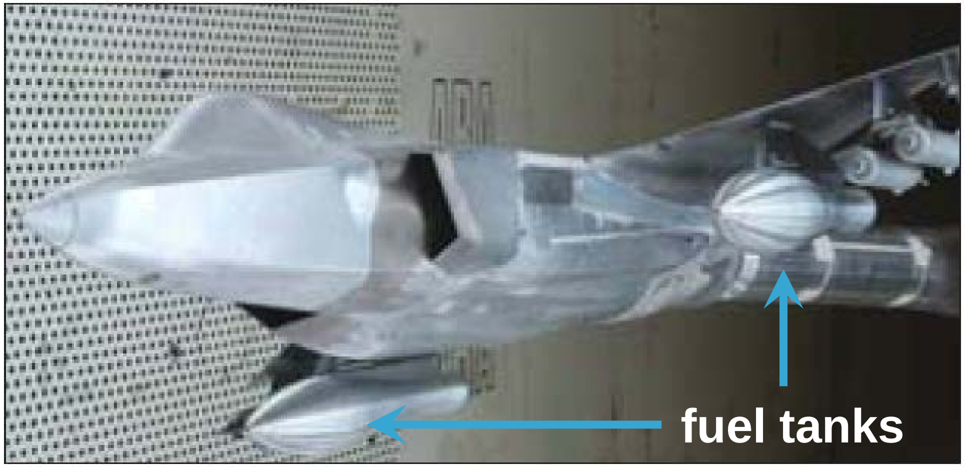


- Device subject to heating, e.g., modeled with heat transfer code
- Uncertainty in composition/ environment (thermal conductivity, density, boundary)
- Make risk-informed decisions about margin to critical temperature



Optimization

- ***Goal-oriented: find the best performing design or scenario, subject to constraints***
  - Identify system designs with maximal performance
  - Determine operational settings to achieve goals
  - Minimize cost over system designs/operational settings
  - Identify best/worst case scenarios

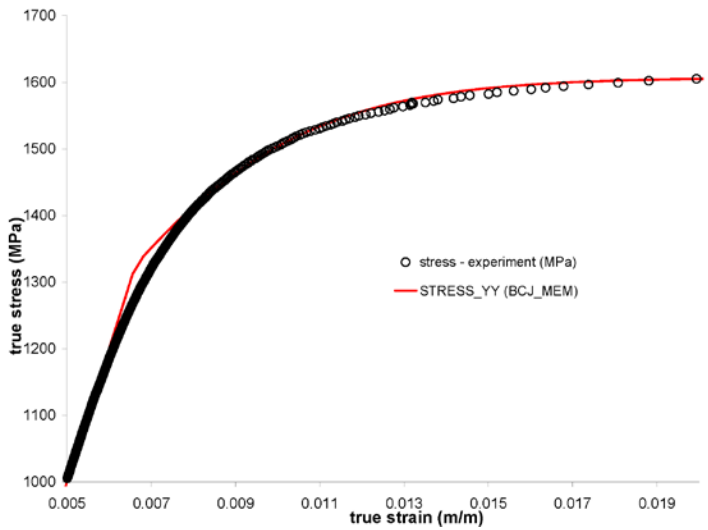


- Computational fluid dynamics code to model F-35 performance
- Find fuel tank shape with constraints to minimize drag, yaw while remaining sufficiently safe and strong

Calibration / Parameter Estimation

- ***Data-driven: find parameter values that maximize agreement between simulation output and experiment***
  - Seek agreement with one or more experiments, or high-fidelity model runs
  - Yields: single best set, range, or distribution of parameters most consistent with data

- Calibrate material model parameters to match experimental stress observations



Dakota: Distinguishing Strengths

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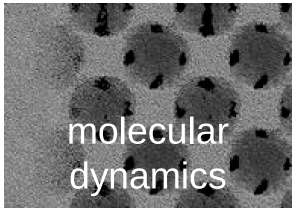
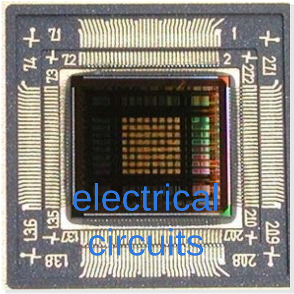
- Makes sensitivity analysis, optimization, and uncertainty quantification practical for costly computational models
- Flexible interface to simulation codes: one interface; many methods
- Combined deterministic/probabilistic analysis
- Continual advanced algorithm R&D to tackle computational challenges (particularly in SNL's national security mission)
  - Treats non-smooth, discontinuous, multi-modal responses
  - Surrogate-based, multi-fidelity, and hybrid methods
  - Risk-informed decision-making: epistemic and mixed UQ, rare events, Bayesian
- Scalable parallel computing from desktop to HPC

What Simulations Work with Dakota?

- Applied to many science and engineering domains:
  mechanics, structures, shock, fluids, electrical, radiation, bio, chemistry, climate, infrastructure, etc.
- Example simulation codes:
  finite element, discrete event, Matlab, Python models

- Helpful simulation characteristics:
  - Can be run in a non-interactive / batch mode
  - Parameters (inputs) not hard-wired, can be adjusted
  - Simulation responses (outputs) can be programmatically processed to extract a few key quantities of interest
  - Model is robust to parameter variations

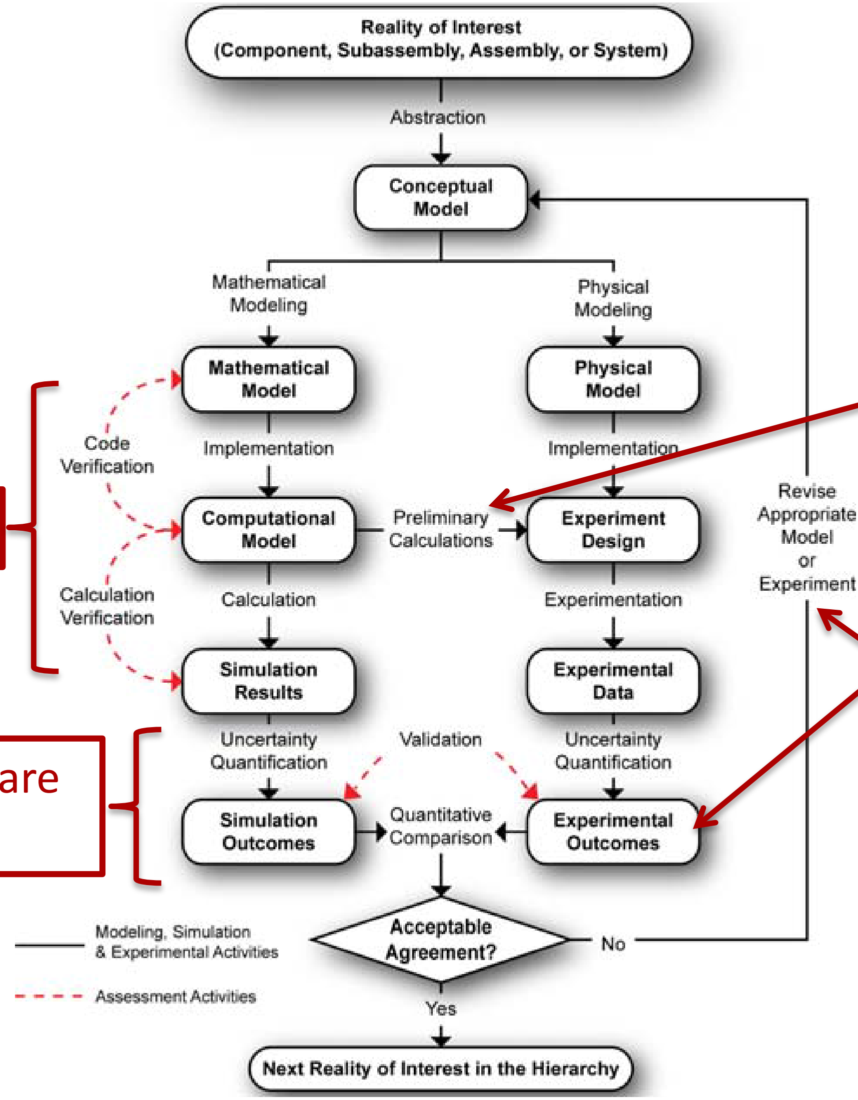




DAKOTA AND VERIFICATION

Supports Overall Simulation Workflow Including Verification and Validation

Enables quantification of margins and uncertainty (QMU) and design with simulations; analogous to experiment-based QMU and physical design/test…



sensitivity analysis to down-select

design of computer experiments

verification

calibration / comparison with data

uncertainty-aware validation

ASME Guide for V&V in Computational Solid Mechanics

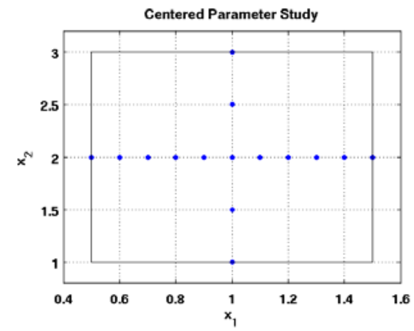
Dakota Verification Methods

- Prerequisite: Simulation exposes numerical parameters, e.g.,
  - Linear/nonlinear solver tolerances
  - Time step or time step control parameters
  - Discretization: knob controlling uniform or adaptive refinement; discrete parameter to select from pre-generated grids
  - Solution algorithm/solver choices
  - (Validation) Model closures, form, discrete selection

- Relevant Dakota Methods
  - Parameter studies
  - Sensitivity analysis
  - Richardson extrapolation
  - *Secondarily: UQ, optimization*

Dakota Verification Methods

- Parameter Studies: see effect of varying knobs
  - Automate manual parameter variation
  - Centered, grid, list



- Sensitivity Analysis: determine critical factors
  - Assess which solution control knobs most affect QoIs
  - Rank numerical knobs to guide verification studies or to find settings that meet computational budget
- Uncertainty Quantification
  - Generate numerical error bars based on solution technique or settings
- Optimization
  - Find mesh quality and solver settings that yield sufficiently resolved results given a computational budget

Richardson Extrapolation

- Basics:
  - Specify numerical controls as continuous state variables with initial values, e.g., char_mesh_size = 4.0
  - Specify refinement rate, e.g., r = 1.5
  - Dakota will evaluate model with a sequence of mesh sizes, e.g., 4.0, 2.7, 1.8, 1.2, …
- Algorithm options:
  - Estimate order: refine twice and estimate order p from 3 grids

$$p = {log\left(\frac{QoI_3 - QoI_2}{QoI_2 - QoI_1}\right)} \Big/ {log(r)}$$

  - Converge order: refine until the convergence order estimate stabilizes
  - Converge QoI: refine until the response QoI converges

APPLICATION EXAMPLES

Cobra-TF Solution Verification

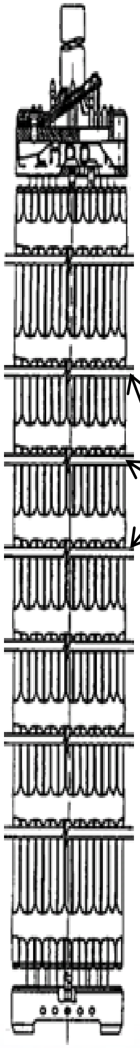
Progression Problem 6 CTF-only

- Initial study produced very good agreement with theoretical expectation (b=0.946 compared to 1.0)
- Problem 6 involves spacer grids of unequal spacing (top & bottom different than interior) requiring meshes characterized by multiple Δz values
- Attempts to lump these into a singe Δz produced poor orders-of-convergence, eg ~0.7 (see report)
- A sensitivity study of total pressure drop on spacer grid locations showed low sensitivity, < 0.2%
- Spacer grid locations were shifted to produce meshes characterized by a single Δz, and the solution verification study was repeated

Axial mesh refinement convergence studies for CTF

Cobra-TF Solution Verification

Progression Problem 6 CTF-only: No Spacer Grids



Omit Spacer Grids

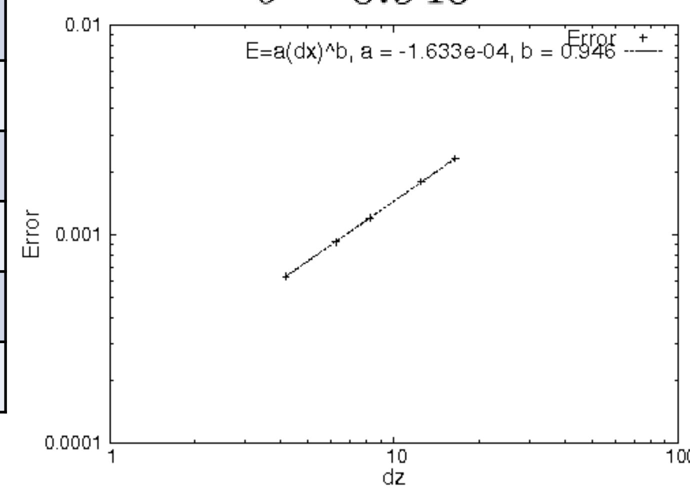
CTF-only Problem 6, No Grids			
Mesh factor, f	Δz (cm)	#Axial elements	Tot. Press. (bar)
0.5	4.160	87	0.68788
0.75	6.240	58	0.68759
1.0	8.225	44	0.68731
1.5	12.479	29	0.68673
2.0	16.450	22	0.68620

Error Model:

$$P = \bar{P} + a\left(\Delta z\right)^b$$

$$E = P - \bar{P} = a\left(\Delta z\right)^b$$

$$b = 0.946$$

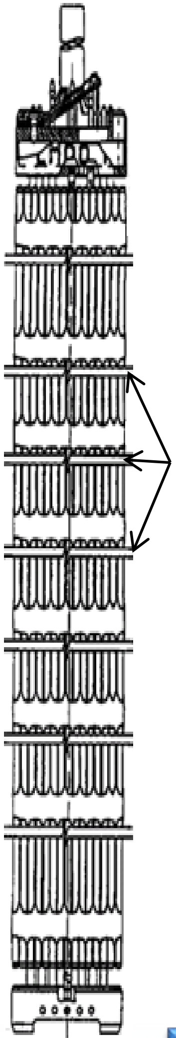


Good agreement with theoretical 1.0

Estimated and theoretical rates consistent: no spacer grids

Cobra-TF Solution Verification

Progression Problem 6 CTF-only: With Spacer Grids*



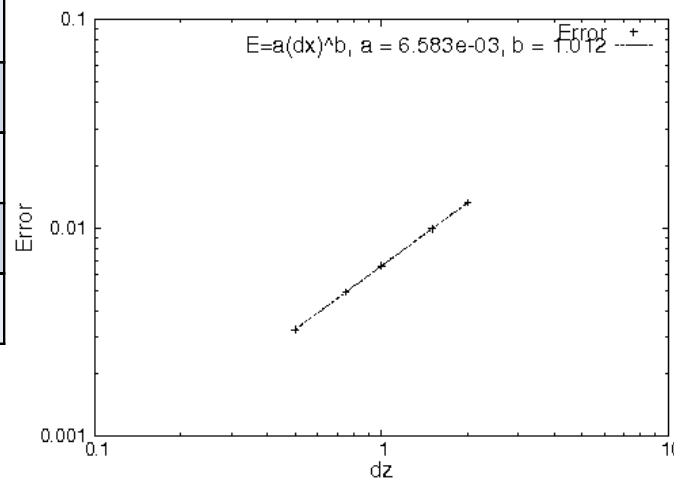
CTF-only Problem 6, With Grids*			
Mesh factor, f	Δz (cm)	#Axial elements	Tot. Press. (bar)
0.5	4.036	72	1.16843
0.75	6.054	48	1.1701
1.0	8.072	36	1.17176
1.5	12.108	24	1.17508
2.0	16.144	18	1.17845

* Grid locations were shifted to produce equal mesh spacing between all grids.

Error Model:

$$E = P - \bar{P} = a\left(\Delta z\right)^{b}$$

$$b = 1.012$$



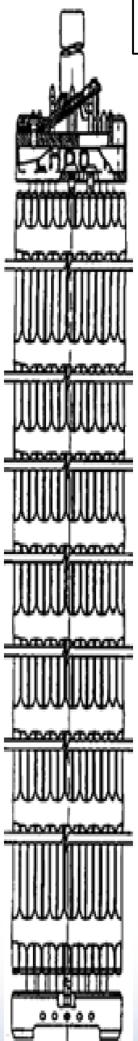
Good agreement with theoretical 1.0

Estimated and theoretical rates consistent with spacer grids

Cobra-TF Solution Verification

Progression Problem 6 CTF-only: With Spacer Grids*

L3:VUQ.V&V.P8.04 “Percept Capabilities in CASL DAKOTA,” March 2014.



Spacer Grid Challenge

* Grid locations were shifted to produce equal mesh spacing between all grids.

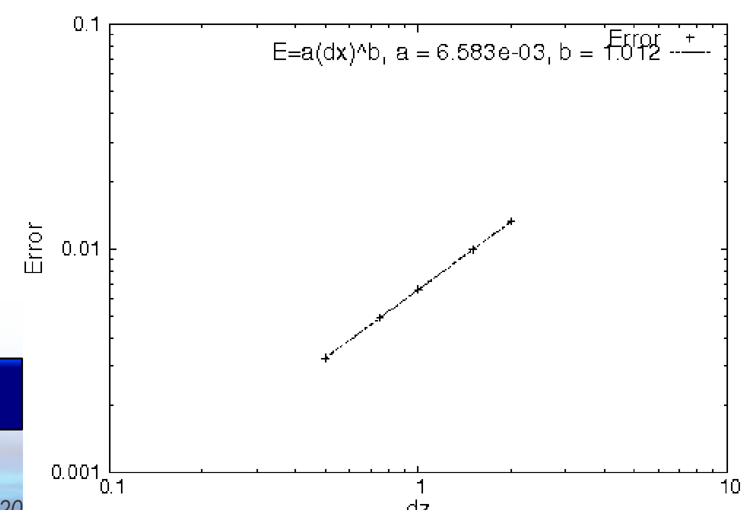
Mesh factor, f	Δz (cm)	#Axial elements	Tot. Press. (bar)
0.5	4.036	72	1.16843
0.75	6.054	48	1.1701
1.0	8.072	36	1.17176
1.5	12.108	24	1.17508
2.0	16.144	18	1.17845

$$E_{(f=1.0)} = 0.0066$$

Error Model:

$$E = P - \bar{P} = a\,(\Delta z)^b$$

$$b = 1.012$$



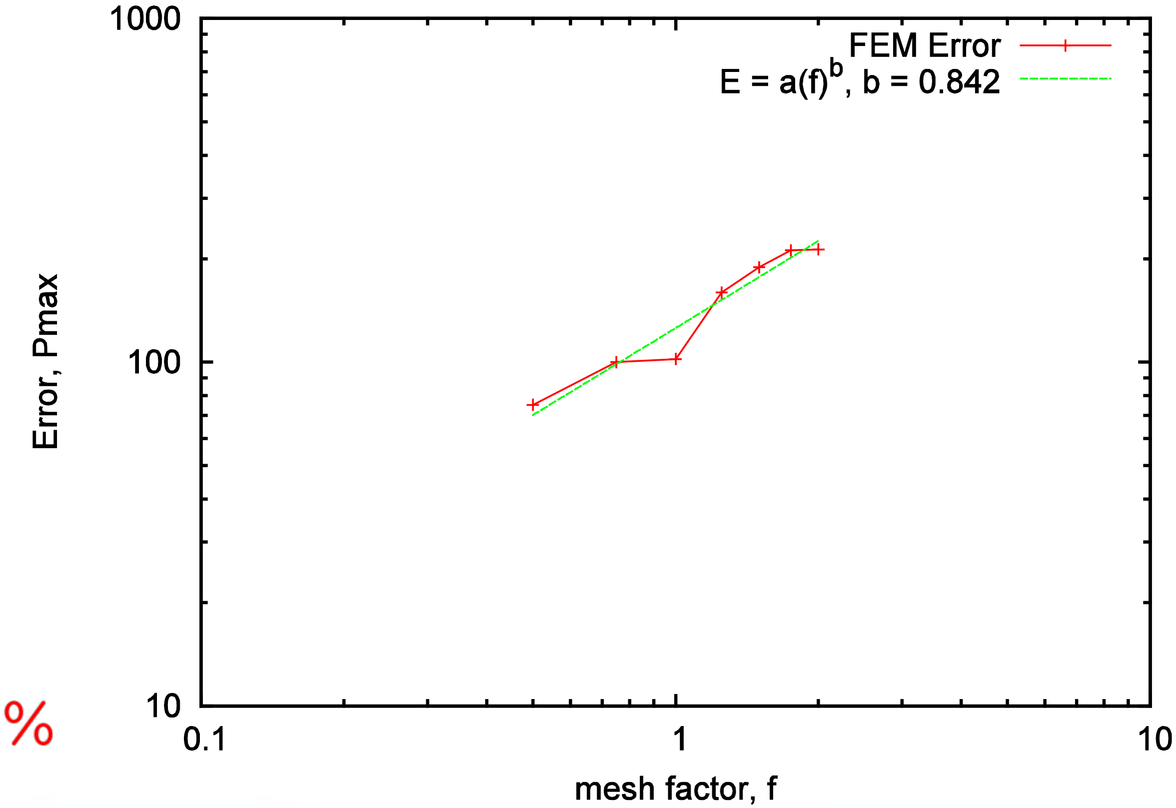
Very good agreement with theoretical 1.0

Fully-Coupled Solution Verification

Progression Problem 6

Each run requires ~600 cpu hours on ORNL's Titan

Progression Problem 6		
Mesh factor, f	#Axial elements	Max Power
0.5	92	27,882
0.75	65	27,907
1.0	50	27,909
1.25	43	27,966
1.5	37	27,995
1.75	35	28,018
2.0	30	28,019



$$E_{(f=1.0)} = 102 = 0.37\%$$

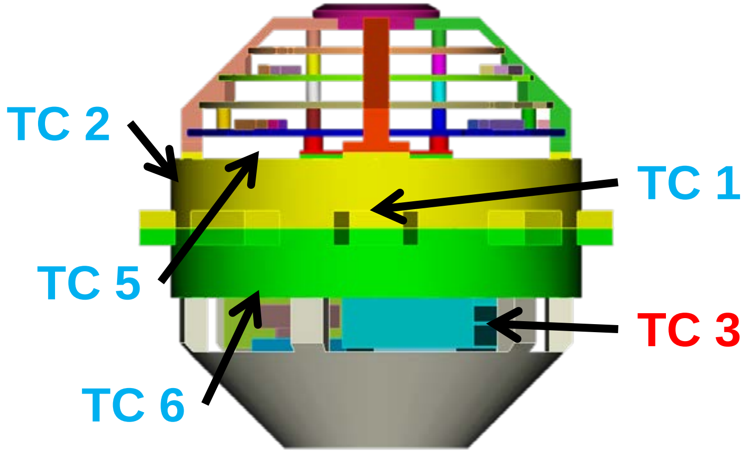
Error Model: $E_{P_{\mathrm{max}}} = P_{\mathrm{max}} - \bar{P}_{\mathrm{max}} = a\,(f)^b$ $\quad b = 0.842$

Degraded order-of-convergence but still usable.

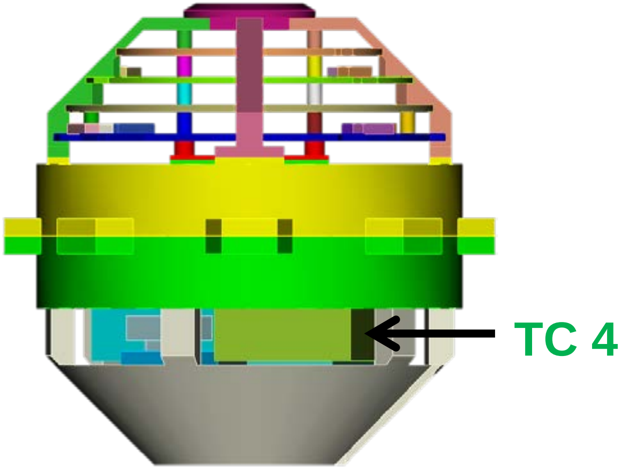
Dakota analyses informed V&V of Ruggedized Instrumentation Package (RIP) model

- System: Assembly of batteries, electronics, and circuit boards in metal housings
- SIERRA Aria Model: Ensure electronics remain within operating temperature range
- 6 Quantities of Interest (QoIs): Temperatures at internal heat sources
  - TC 1,2,5,6 are located on the battery housing
  - TC 3 and TC 4 are located on electronics packages
- Dakota used to
  - Examine sensitivity to 27 numerical parameters
  - Examine sensitivity to 57 model parameters
  - Propagate uncertainty for comparison to experiment

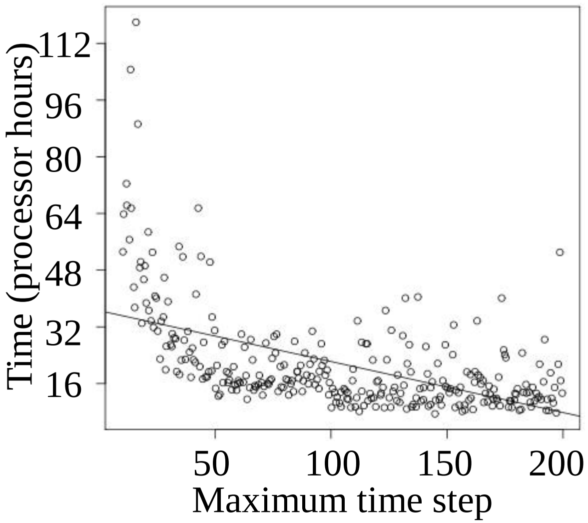
Front View



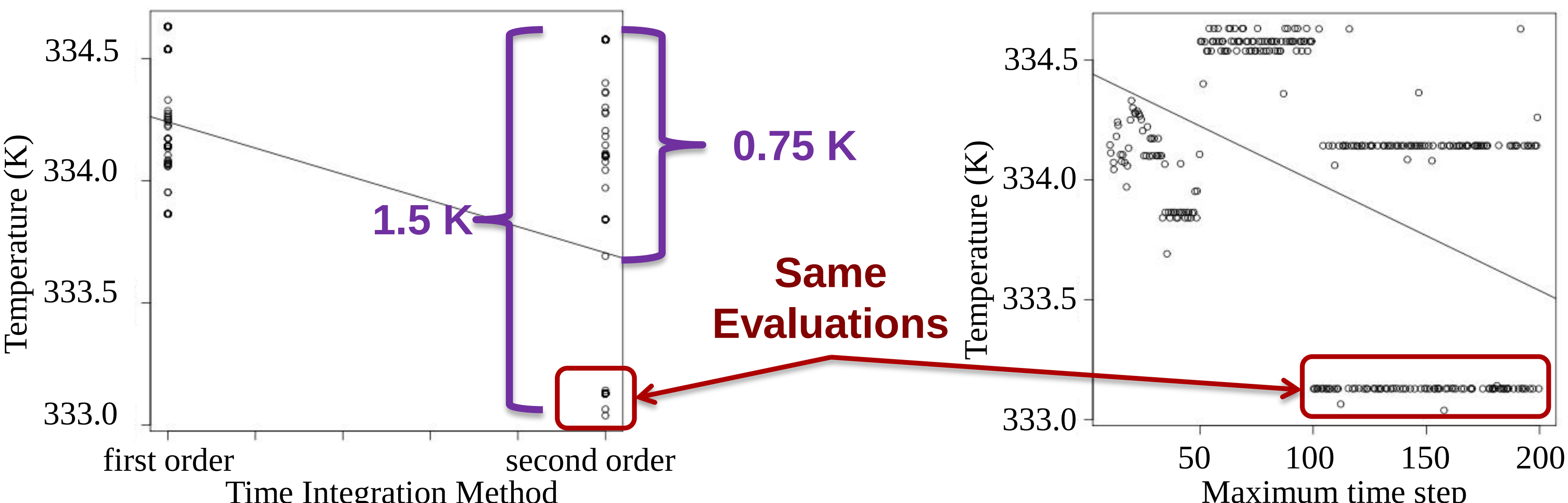
Back View



Dakota sensitivity studies identified tradeoffs between QoI variability and simulation time



Temperature variability can be reduced by setting the max time step to 50 or below without increasing simulation time



S.N. Scott, J.A. Templeton, P. D. Hough, J. R. Ruthruff, M.V. Rosario, J.P. Peterson, "Statistical Validation For Heat Transfer Problems: A Case Study", *International Journal of Computational Methods and Experimental Measurements*, Volume 3 (2015), Issue 2, Pages 101–120.

Dakota History and Resources

- Genesis: 1994 optimization LDRD
- Modern software quality and development practices
- Released every May 15 and Nov 15
- Established support process for SNL, partners, and beyond

Mike Eldred, Founder

Lab mission-driven algorithm R&D deployed in production software

- Extensive website: documentation, training materials, downloads
- Open source facilitates external collaboration; widely downloaded

Engaging Dakota

Algorithms for Design Exploration and Uncertainty Quantification

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Website: http://dakota.sandia.gov

- Download (LGPL license, freely available worldwide)
- Getting Started guide; User's Manual: Tutorial with example input files
- Extensive documentation (user, reference, developer)
- Support mailing list (reaches both Dakota team and user community)

In CASL

- Available in VERA
- CASL/Dakota User's Manual (on Dakota publications page)
- People resources
  - Brian Williams, Ralph Smith
  - Vince Mousseau, Natalie Gordon, Lindsay Gilkey
  - Westinghouse, EPRI users

Thanks for your attention! *briadam@sandia.gov, rhoope@sandia.gov*